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Estimates of Logarithmic Sobolev Constant: An Improvement of Bakry–Emery Criterion*

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This paper is mainly devoted to estimate the logarithmic Sobolev (abbrev. L.S.) constant for diffusion operators on manifold or in $\mathbb{R}^d$. In most cases, we study

Anal. **92** (1990), 30–48]) of the comparison between the L.S. constants for different potentials, the powerful Bakry–Emery criterion for the L.S. inequality is improved considerably in the paper, especially for the manifolds with non-positive sectional curvatures (Theorem 1.3(1)). In terms of our notation: $\beta(r)=\inf_{\rho(x,p)\geqslant r}\inf_{X\in T_x(M),\,\|X\|=1}(\mathrm{Ricc}-\mathrm{Hess}_V)(X,X)$, where $\rho(x,p)$ is the distance between x and an arbitrary fixed point $p\in M$, the improvement can be roughly stated as follows. The condition "$\inf_{r\geqslant 0}\beta(r)>0$" for which the criterion is available is now replaced by "$\sup_{r\geqslant 0}\beta(r)>0$." © 1997 Academic Press

1. MAIN RESULTS AND EXAMPLES

Let (M,g) be a d-dimensional, connected, complete Riemannian manifold and let Ω be a compact and convex regular domain of M. Suppose that $\mathrm{Ricci}\geqslant Kg$ on M for some constant $K\in\mathbb{R}$. Next, let $L=\Delta+\nabla V$, $V\in C^2(\Omega)$. Consider the reflecting L-diffusion process with reversible measure $d\mu=e^V\,d\lambda/Z$, where λ is the Riemannian volume element and $Z=\int_\Omega e^V\,d\lambda$ (cf. [10]). Since Ω is compact, the following logarithmic Sobolev inequality (Gross [7])

$$\int_\Omega f^2\log f^2\,d\mu\leqslant\frac{2}{\alpha}\int_\Omega\|\nabla f\|^2\,d\mu \tag{1.1}$$

holds for some constant $\alpha>0$ and for all $f\in C^1(\Omega)$ with $\mu(f^2):=\int_\Omega f^2\,d\mu=1$. The largest constant α, denoted by $\alpha_\Omega(V)$, is called the L.S.

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constant. The inequality has a very wide range of applications. Refer to the survey article [8] for the history and the current states of the study on the topic.

One powerful method to deduce the inequality is the Bakry–Emery (abbrev. B.-E.) criterion [2] which has been reexamined and improved by many authors (refer to [1] and [4] for details and references therein). For instance, Deuschel and Stroock [5; Remark 1.20] mentioned the following comparison between the L.S. constants for different potentials V and U:

$$\alpha_\Omega(V) \geqslant \alpha_\Omega(U) \exp[-\operatorname{osc}_\Omega(V-U)], \tag{1.2}$$

where $\operatorname{osc}_\Omega(V) = \sup_\Omega V - \inf_\Omega V$ (The negative sign in the exponential was missed in [5; (1.21)]). This is a starting point of the paper. To check (1.2), simply use the identity

$$\int_\Omega f \log \frac{f}{\mu(f)}\, d\mu = \inf\left\{\int_\Omega (f \log f - f \log t - f + t)\, d\mu \colon t \in (0, \infty)\right\}$$

for all strictly positive and smooth f and note that the integrand on the right-hand side is non-negative for all $t \in (0, \infty)$. At the first look, (1.2) seems quite rough but it does yield sharp estimates as we will see in Corollary 1.6 and examples below. On the other hand, it was proved in [5] and [11] that

$$\alpha_\Omega(V) \geqslant K_\Omega(V) + d^{-1}\lambda_1(0)\, e^{-\operatorname{osc}_\Omega(V)}, \tag{1.3}$$

where

$$K_\Omega(V) = \inf\{(\mathrm{Ric} - \mathrm{Hess}_V)(X, X) \colon X \in T_x M,\ \|X\| = 1,\ x \in \Omega\}$$

and $\lambda_1(V)$ is the spectral gap (=the first non-trivial eigenvalue) of the reflecting L-diffusion on Ω (see [10] for some detailed estimates of $\lambda_1(V)$). Actually, $\lambda_1(V)$ is the largest constant λ for which the Poincaré inequality

$$\int_\Omega (f - \mu(f))^2\, d\mu \leqslant \frac{1}{\lambda} \int_\Omega \|\nabla f\|^2\, d\mu, \qquad f \in C^1(\Omega)$$

holds. A well-known fact is that $\lambda_1(V) \geqslant \alpha_\Omega(V)$. When $K > 0$, the estimate (1.3) can be sharp in the free boundary situation [5], but they are ineffective for sufficient small K. Thus, we will concentrate on the case of small K (especially, $K \leqslant 0$).

Let ρ be the Riemannian distance induced by g. Fixed $p \in \Omega$ and set $D = \sup_\Omega \rho(x, p)$. Denote by $C(p)$ the cut locus of p. Define

$$\tilde{\Omega} = \{x \in M\text{: there exists } y \in \Omega \text{ such that } x \text{ belongs to the shortest geodesic from } p \text{ to } y\}.$$

Now, as an addition to [5] and [11], we have the following result.

THEOREM 1.1. *Suppose that $\Omega \cap C(p) = \emptyset$ and the sectional curvatures of $\tilde{\Omega}$ are bounded above by a constant $k \in \mathbb{R}$. Then*

$$\alpha_\Omega(V) \geqslant \sup_{\beta > 0} \left(\alpha_\beta + d^{-1} e^{-\beta D^2} \lambda_1(0)\right) e^{-\operatorname{osc}_\Omega(V + \beta\rho(\cdot, p)^2)},$$

where

$$\alpha_\beta = \begin{cases} K + 2\beta, & \text{if } \ k \leqslant 0 \\ K + 2\sqrt{k}\, D \operatorname{ctan}(\sqrt{k}\, D)\, \beta, & \text{if } \ k > 0 \ \text{ and } \ 2\sqrt{k}\, D < \pi. \end{cases}$$

The proof of the theorem is based on the Hessian comparison theorem (see (2.1) and (2.2) in the next section). From which the restriction "$2\sqrt{k}\, D < \pi$" in the last line arises. The next result is a simple consequence of Theorem 1.1.

COROLLARY 1.2. *Under the assumptions of Theorem* 1.1, *we have*

$$\alpha_\Omega(V) \geqslant \begin{cases} e^{-\operatorname{osc}_\Omega(V)} \left\{ \dfrac{2}{D^2} \exp\left[-1 + \dfrac{KD^2}{2}\right] \right. \\ \quad \left. + \dfrac{\lambda_1(0)}{d} \exp[-2 + KD^2] \right\}, \qquad \text{if } \ k \leqslant 0 \\ e^{-\operatorname{osc}_\Omega(V)} \left\{ \dfrac{2\sqrt{k}}{D \tan(\sqrt{k}\, D)} \exp\left[-1 + \dfrac{KD\tan(\sqrt{k}\, D)}{2\sqrt{k}}\right] \right. \\ \quad \left. + \dfrac{\lambda_1(0)}{d} \exp\left[-2 + \dfrac{KD\tan(\sqrt{k}\, D)}{\sqrt{k}}\right] \right\}, \\ \quad \text{if } \ 0 < k \leqslant \dfrac{\pi^2}{4D^2} \ \text{ and } \ \dfrac{\sqrt{k}}{\tan(\sqrt{k}\, D)} > \dfrac{KD}{2}. \end{cases}$$

Next, we go to the free boundary case. We consider the non-compact manifold only since in the compact case the same topic was treated in [5] and [11]. Again, we will use the comparison (1.2) which also holds in the present situation. However, the potential now becomes more essential, without it, $\alpha(L)$ can be vanished. Hence, to produce a good estimate, the potential U has to be carefully designed especially for unbounded manifold (see also the remark right after the proof of Theorem 1.3).

Consider the operator having the form $L = \Delta + \nabla V$ and assume that its Dirichlet form is regular. Replacing Ω in (1.1) by the whole space M, we obtain the L.S. inequality for L and then we have the constants $\alpha(V) := \alpha_M(V)$ and $K(V) := K_M(V)$. Next, define

$$K(V, x) = \inf\{(\mathrm{Ric} - \mathrm{Hess}_V)(X, X) \colon X \in T_x M,\ \|X\| = 1\}, \qquad x \in M.$$

Clearly, $K(V) = \inf_x K(V, x)$. Note that in the most interesting (non-compact) cases, $\mathrm{osc}(V) = \infty$ and so the criterion (1.3) becomes $\alpha(V) \geqslant K(V)$. Fix $p \in M$ and let $\beta(r) = \inf_{\rho(x,p) \geqslant r} K(V, x)$. Obviously, $\beta(r)$ is increasing in r. Moreover, $\beta(0) = \inf_{r \geqslant 0} \beta(r) = K(V)$. For fixed $k \geqslant 0$, define $f(r) = r$ if $k = 0$ and $f(r) = \sin(\sqrt{k}\, r)/\sqrt{k}$ if $k > 0$. Set $\tilde{\beta}(r) = \inf_{u \colon f(u) \in [r, \pi/(2\sqrt{k}))} \beta(u)/f'(u)$. Here and in what follows, $1/\sqrt{k}$ is understood as ∞ when $k = 0$. Note that $\tilde{\beta}(r) = \beta(r)$ when $k = 0$ since β is an increasing function. Finally, for fixed $a \in [0, \pi/(2\sqrt{k}))$, define

$$\gamma(r) = \frac{1}{f(r)} \int_0^{f(r)} \tilde{\beta}(u)\, du, \qquad r < \frac{\pi}{2\sqrt{k}}$$

and

$$F_a(r) = \int_0^{r \wedge a} ds \int_0^{f(s)} [\gamma(a) - \tilde{\beta}(u)]\, du, \qquad r \geqslant 0. \tag{1.4}$$

We can now state the main result of the paper.

THEOREM 1.3. *Suppose that the sectional curvatures of M are bounded above by a constant $k \in \mathbb{R}$.*

(1) *Let $k = 0$. If $M \cap C(p) = \varnothing$ and $\sup_{r \geqslant 0} \beta(r) > 0$, then we have*

$$\alpha(V) \geqslant \frac{2}{a_0^2} \exp\left[1 - \int_0^{a_0} r\beta(r)\, dr\right] > 0, \tag{1.5}$$

where $a_0 > 0$ is the unique solution to the equation $\int_0^a \beta(r)\, dr = 2/a$.

(2) *Let $k > 0$. If $C(p) \cap B(p, \pi/(2\sqrt{k})) = \varnothing$ and $\gamma(a) > 0$ for some $a \in (0, \pi/(2\sqrt{k}))$, then we have $\alpha(V) \geqslant f'(a)\, \gamma(a) \exp[-F_a(a)] > 0$.*

When $k = 0$, the B.-E. criterion requires that $\inf_{r \geqslant 0} \beta(r) > 0$. From this, one sees that the criterion is now improved considerably by Theorem 1.3(1). Actually, as we will prove in the next section (see (2.5)), the lower bound given in (1.5) always dominates $\beta(0)$. Besides, note that the L.S. inequality is based on a kind of (uniform) ergodicity, which requires a limiting behavior of the potential when $\rho(x, p) \to \infty$. From this point of view, our condition "($\lim_{r\to\infty} \beta(r) =$) $\sup_{r \geqslant 0} \beta(r) > 0$" seems reasonable.

We now turn to study the multi-dimensional diffusion processes. Let

$$L = \sum_{i,j=1}^{d} a_{ij}(x) \frac{\partial^2}{\partial x_i \, \partial x_j} + \sum_{i=1}^{d} b_i(x) \frac{\partial}{\partial x_i},$$

where $a(x) = (a_{ij}(x))$ is positive definite, $a_{ij} \in C^2(\mathbb{R}^d)$ and

$$b_i(x) = \sum_{j=1}^{d} a_{ij}(x) \frac{\partial}{\partial x_j} V(x) + \sum_{j=1}^{d} \frac{\partial}{\partial x_j} a_{ij}(x)$$

for some $V \in C^2(\mathbb{R}^d)$ with $Z := \int e^V dx < \infty$. The specific form of b_i implies that the L-diffusion process is reversible with respect to $d\mu = Z^{-1} e^V dx$ (see [3]). In the present context, the L.S. inequality becomes

$$\int_{\mathbb{R}^d} f^2 \log f^2 \, d\mu \leqslant \frac{2}{\alpha(L)} \int_{\mathbb{R}^d} \langle a \, \nabla f, \nabla f \rangle \, d\mu \tag{1.6}$$

for all bounded $f \in C^2$ with $\mu(f^2) = 1$, where $\langle \cdot, \cdot \rangle$ is the Euclidean inner product. Here we have used $\alpha(L)$ rather than $\alpha(V)$ to denote the L.S. constant which now depends on the whole coefficients of L, not only on the potential V. Certainly, by using the Riemannian metric $g = a(x)^{-1}$, one can regard the present situation as a special case of what treated above. However, in general, both the Riemannian distance and the Ricci curvature are too complex to be computed. To avoid doing so, we adopt the idea of [3] to simplify the operator by a comparison argument (see the proof of Corollary 1.4 for details). In this way, we obtain the following simple consequence of Theorem 1.3(1).

COROLLARY 1.4. *Suppose that $a(x) \geqslant \delta \sigma^2$ for some $\delta > 0$ and a positive definite constant matrix σ. Let $\lambda_V(x)$ be the largest eigenvalue of the matrix $\sigma(\partial^2 V(x)/\partial x_i \, \partial x_j) \, \sigma$ and let $\bar\beta(r) = \inf_{|\sigma^{-1}(x-p)| \geqslant r} \{-\lambda_V(x)\}$ for fixed $p \in \mathbb{R}^d$. If $\sup_{r \geqslant 0} \bar\beta(r) > 0$, then we have*

$$\alpha(L) \geqslant \frac{2\delta}{a_0^2} \exp\left[1 - \int_0^{a_0} r \bar\beta(r) \, dr\right] > 0,$$

where $a_0 > 0$ is the unique solution to the equation $\int_0^a \bar\beta(r) \, dr = 2/a$.

Finally, we go to study the upper bound of the L.S. constant. As was mentioned above, the spectral gap already provides a upper bound for $\alpha(L)$. A different approach is provided by the following result which is a generalization to [9; Theorem 1].

THEOREM 1.5. *Suppose that* $a(x) \leqslant v(x)\,\bar{a}(x)$ *for some non-negative* $v \in C(\mathbb{R}^d)$ *and a matrix* $\bar{a}(x)$ *with continuous components and having the property: there exist constants* $\bar{v}_1, \bar{v}_2 > 0$ *such that* $\bar{v}_1 I \leqslant \bar{a}(x) \leqslant \bar{v}_2 I$. *Let* $\gamma_n = \inf_{|x| \geqslant n}[-V(x)]$. *If* $\gamma_n > 0$ *for large n,* $\lim_{n\to\infty} \gamma_n^{-1} \log n = 0$ *and there exists a constant C such that* $|V(x)|/\|\nabla V(x)\| \leqslant C\,|x|$ *for large* $|x|$, *then we have*

$$\alpha(L) \leqslant \tfrac{1}{2} \varlimsup_{|x|\to\infty} \left[-\langle \bar{a}(x)\,\nabla V(x), \nabla V(x)\rangle\, v(x)/V(x)\right].$$

We mention that by some slight modifications, Theorem 1.5 can be also extended to a class of manifolds whose volume grows no more faster than a polynomial of the diameter. Combining Corollary 1.4 with Theorem 1.5, we can get the exact value of $\alpha(L)$ for some particular operators, as illustrated below.

COROLLARY 1.6. *Suppose that* $\delta\sigma^2 \leqslant a(x) \leqslant v(x)\,\sigma^2$ *for some constant* $\delta > 0$, *positive definite matrix* σ *and* $v(x) \in C(\mathbb{R}^d)$ *with* $\lim_{|x|\to\infty} v(x) = \delta$. *Take* $V(x) = -b\,|x|^2/2$, $b > 0$. *Then we have* $\delta b \lambda_{\min}(\sigma)^2 \leqslant \alpha(L) \leqslant \delta b \lambda_{\max}(\sigma)^2$.

The lower bound here coincides with the one of $\lambda_1(L)$ given in [3]. Once σ has a unique eigenvalue, we obtain the exact $\alpha(L)$ for a large class of $a(x)$. To conclude this section, we discuss some examples.

EXAMPLE 1.7. Consider the domain $[0, \infty)$ and take $a(x) \equiv 1$, $V(x) = -bx$ $(b > 0)$. By Theorem 1.5, we have $\alpha(L) = 0$. This means that for the operator with constant diffusion coefficient, the L.S. inequality holds only when the potential V decays faster than linear. However, for this example, we have $\lambda_1(L) = b^2/4$ (see [3]).

EXAMPLE 1.8 [9]. Take $M = (0, \infty)$, $a(x) = x$ and $b(x) = -(x - b)$, $b > 0$. Applying Theorem 1.3(1) to $g(d/dx, d/dx) = x^{-1}$, we get $\alpha(L) \geqslant 1/2$ whenever $b \geqslant 1/2$. In view of Theorem 1.5, this estimate is exact when $b \geqslant 1/2$.

It is interesting that for this example the Riemannian and the Euclidian metrics provide us respectively the sharp estimates of $\alpha(L)$ and $\lambda_1(L)$ $(=1$ for all $b > 0$ [3]), but not conversely.

EXAMPLE 1.9. Take $\Omega = [a, b] \subset \mathbb{R}$. By setting $\beta = 0$ in Theorem 1.1, we obtain

$$\alpha_\Omega(V) \geqslant \lambda_1(0)\, e^{-\operatorname{osc}_\Omega(V)} = \frac{\pi^2}{(b-a)^2}\, e^{-\operatorname{osc}_\Omega(V)}. \qquad \text{(cf. [10])}$$

In particular, $\alpha_\Omega(0) = \lambda_1(0) = \pi^2/(b-a)^2$ since $\alpha_\Omega(0) \leqslant \lambda_1(0)$.

The next two examples illustrate that Corollary 1.4 does improve the B.-E. criterion.

EXAMPLE 1.10. Take $d=1$, $a(x)=(1+x^2)^2$ and $V(x)=-vx^2/2$, $v>0$. Applying Corollary 1.4 to $\delta=1$, $\lambda_V(x)\equiv -v$ and $\bar{\beta}(r)\equiv v$, we obtain $\alpha(L)\geqslant v$.

On the other hand, let $g(d/dx, d/dx)=(1+x^2)^{-2}$, then $L=\Delta_g+\nabla_g[-vx^2/2+\log(1+x^2)]=: \Delta_g+\nabla_g \bar{V}$. We have

$$\operatorname{Hess}_{\bar{V}}\left((1+x^2)\frac{d}{dx}, (1+x^2)\frac{d}{dx}\right)$$

$$=\left[(1+x^2)\frac{d}{dx}\right]^2 \bar{V}=-v(1+x^2)(1+3x^2)+2(1+x^2).$$

Hence, the B.-E. criterion gives us

$$\alpha(L)\geqslant \inf_x \left[v(1+x^2)(1+3x^2)-2(1+x^2)\right]=v-2$$

provided $v\geqslant 1/2$, otherwise, the infimum is negative. Therefore, the criterion is available only if $v>2$.

In contrast to Example 1.8, here the Euclidian metric produces a better estimate for $\alpha(L)$ rather than the Riemannian one.

EXAMPLE 1.11. Take $a(x)\equiv I$ and $V(x)=-|x|^4+v\,|x|^2$ $(v\geqslant 0)$. We have $\partial^2 V/\partial x_i\,\partial x_j=-8x_ix_j+(2v-4\,|x|^2)\,\delta_{ij}$. That is, $(\partial^2 V/\partial x_i\,\partial x_j)=-8xx^*+(2v-4\,|x|^2)\,I$. For $p=0$ we have $\beta(r)=4r^2-2v$ if $d\geqslant 2$ and $\beta(r)=12r^2-2v$ if $d=1$. By Theorem 1.3 or Corollary 1.4, we get

$$\alpha(L)\geqslant\begin{cases}\dfrac{8}{3v+\sqrt{3(3v^2+8)}}\exp\left[-\dfrac{3v^2+4+v\sqrt{3(3v^2+8)}}{8}\right], & \text{if } d\geqslant 2\\[2ex] \dfrac{8}{v+\sqrt{v^2+8}}\exp\left[-\dfrac{v^2+4+v\sqrt{v^2+8}}{8}\right], & \text{if } d=1.\end{cases}$$

In particular, when $v=0$, we have $\alpha(L)\geqslant 2\sqrt{2/3}\,e^{-1/2}>0.99$ if $d\geqslant 2$ and $\alpha(L)\geqslant 2\sqrt{2}\,e^{-1/2}>1.71$ if $d=1$, which are better than the lower bound of the spectral gap given in [3]. When $d=1$, the test function $f(x)=x$ gives us $\alpha(L)\leqslant\lambda_1(L)<2.96$. However, the B.-E. criterion is not available for this example since $\beta(0)=-2v\leqslant 0$.

EXAMPLE 1.12. Take $d=1$, $a(x)\equiv 1$ and $V(x)=-x^2/2+2\sin x$. Then $\beta(r)\equiv -1$ and so Theorem 1.3 is not suitable. However, applying (1.2) to

$V(x) = -x^2/2$ and $V(x) - U(x) = 2\sin x$, we have $\alpha(L) \geqslant e^{-2}$. This means that the condition "$\sup_{r \geqslant 0} \beta(r)$" is still not necessary for the L.S. inequality and a bounded perturbation should be carefully treated before applying Theorem 1.3.

2. PROOFS

Proof of Theorem 1.1. Set $\rho(x) = \rho(x, p)$. For $x \in \Omega$, let γ: $[0, \rho(x)] \to \tilde{\Omega}$ be the unique shortest geodesic from p to x. Let M_k be a simply connected d-dimensional manifold with constant sectional curvature k. Choose $\tilde{p}$ and $\tilde{x} \in M_k$ such that $\tilde{\rho}(\tilde{p}, \tilde{x}) = \rho(x)$. By assumption, either $k \leqslant 0$ or $k > 0$ but still $2\sqrt{k}\,\rho(x) < \pi$, we have $\tilde{x} \notin C(\tilde{p})$. For $X \in T_x M$ with $\|X\| = 1$, take $\tilde{X} \in T_{\tilde{x}} M_k$ so that $\|\tilde{X}\| = 1$ and $X\rho(x) = \tilde{X}\tilde{\rho}(\tilde{p}, \cdot)(\tilde{x})$. By Hessian comparison theorem [6, 12], we have

$$\mathrm{Hess}_\rho(X, X) \geqslant \mathrm{Hess}_{\tilde{\rho}(\tilde{p}, \cdot)}(\tilde{X}, \tilde{X}) = (f'/f)(\rho(x))(1 - (X\rho(x))^2), \quad (2.1)$$

where

$$f(r) = \begin{cases} r, & \text{if } k = 0 \\ \sinh(\sqrt{-k}\, r)/\sqrt{-k}, & \text{if } k < 0 \\ \sin(\sqrt{k}\, r)/\sqrt{k}, & \text{if } k \in (0, \pi/(2\sqrt{k})). \end{cases} \quad (2.2)$$

For $x \in \Omega$ and $X \in T_x M$ with $\|X\| = 1$, since $(X\rho)^2 \leqslant \|X\|^2 = 1$, by (2.1), we have

$$\begin{aligned} \mathrm{Hess}_{\rho^2}(X, X) &= 2\rho\, \mathrm{Hess}_\rho(X, X) + 2(X\rho)^2 \\ &\geqslant \begin{cases} 2, & \text{if } k \leqslant 0 \\ 2\sqrt{k}\, D \,\mathrm{ctan}(\sqrt{k}\, D), & \text{if } k > 0. \end{cases} \end{aligned}$$

Therefore $K_\Omega(-\beta\rho^2) \geqslant \alpha_\beta$. By (1.3), we get

$$\alpha_\Omega(-\beta\rho^2) \geqslant \alpha_\beta + d^{-1}\lambda_1(0)\, e^{-\mathrm{osc}_\Omega(-\beta\rho^2)} = \alpha_\beta + d^{-1}\lambda_1(0)\, e^{-\beta D^2}.$$

Now, Theorem 1.1 follows from (1.2). ∎

Proof of Corollary 1.2. Note that $\mathrm{osc}_\Omega(V + \beta\rho^2) \leqslant \mathrm{osc}_\Omega(V) + \beta D^2$, by Theorem 1.1, we have

$$\alpha_\Omega(V) \geqslant e^{-\mathrm{osc}_\Omega(V)} \sup_{\beta > 0} e^{-\beta D^2}[\alpha_\beta + d^{-1}\lambda_0(0)\, e^{-\beta D^2}].$$

Then, the desired estimates are obtained by choosing

$$\beta=\begin{cases}\dfrac{1}{D^2}-\dfrac{K}{2}, & \text{if} \quad k\leqslant 0\\[2ex] \dfrac{1}{D^2}-\dfrac{K\tan(\sqrt{k}\,D)}{2\sqrt{k}\,D}, & \text{if} \quad k>0.\end{cases}$$

Here we have used the condition that $\sqrt{k}/\tan(\sqrt{k}\,D)>KD/2$. ∎

Proof of Theorem 1.3. (1) First, we prove part (1) of Theorem 1.3.

(a) Let $\sup_{r\geqslant 0}\beta(r)>0$. Then, we have $\beta(0)>-\infty$. Since $k=0$ and $f(r)=r$, from (1.4), it follows that $\gamma(r)=(1/r)\int_0^r\beta(s)\,ds$, $r>0$, $\gamma(0)=\beta(0)$ and

$$C_a(r)=[\gamma(a)-\beta(r)]\,I_{[r\leqslant a]},\quad a\geqslant 0,\qquad F_a(r)=\int_0^r ds\int_0^s C_a(u)\,du,\quad r\geqslant 0.$$

Note that $\beta(r)$ is increasing in r and so is $\gamma(r)$. Next, let $G(a)=\gamma(a)\exp[-F_a(a)]$ for simplicity. We will prove the following two assertions:

$$\alpha(V)\geqslant\sup_{a\geqslant 0}G(a). \tag{2.3}$$

and

$$\sup_{a\geqslant 0}G(a)=G(a_0) \tag{2.4}$$

where $a_0>0$ is determined uniquely by the equation $\int_0^a\beta(r)\,dr=2/a$. These assertions certainly imply the statement of Theorem 1.3: $\alpha(V)\geqslant G(a_0)$. We now prove the second assertion. Note that

$$\begin{aligned}F_a(a)&=\int_0^a dr\int_0^r[\gamma(a)-\beta(s)]\,ds=\frac{a^2}{2}\gamma(a)-\int_0^a dr\int_0^r\beta(s)\,ds\\&=\frac{a^2}{2}\gamma(a)-\int_0^a\gamma(r)\,d\left(\frac{r^2}{2}\right)=\frac{1}{2}\int_0^a r^2\gamma'(r)\,dr.\end{aligned}$$

Hence $G'(a)=\gamma'(a)[1-a^2\gamma(a)/2]\exp[-F_a(a)]$. Because $\gamma'\geqslant 0$ and the uniqueness of a_0, we have $G'\geqslant 0$ on $[0,a_0]$ and $G'\leqslant 0$ on $[a_0,\infty)$. Thus, the global maximum of G is achieved at a_0. This proves (2.4). Next, since $a_0^2\gamma(a_0)=2$, we have

$$\begin{aligned}F_{a_0}(a_0)&=\frac{a_0^2}{2}\gamma(a_0)-\int_0^{a_0}dr\int_0^r\beta(s)\,ds=1-\int_0^{a_0}(a_0-s)\,\beta(s)\,ds\\&=1-a_0^2\gamma(a_0)+\int_0^{a_0}r\beta(r)\,dr=-1+\int_0^{a_0}r\beta(r)\,dr.\end{aligned}$$

Thus, $G(a_0)$ coincides with the lower bound given in (1.5). Moreover,

$$G(a_0) = \sup_{a \geqslant 0} G(a) \geqslant G(0) = \beta(0), \tag{2.5}$$

which was mentioned in the last section.

(b) We now begin to prove (2.3). Since we always have $\alpha(V) \geqslant 0$, (2.3) is meaningful iff $\sup_{a \geqslant 0} \gamma(a) > 0$ (equivalently, $\sup_{r \geqslant 0} \beta(r) > 0$). Thus, by (a), we need only to show that $\alpha(V) \geqslant G(a_0)$. But the proof given below makes no difference if we replace a_0 with any fixed $a > 0$. Because

$$F'_a(r) = \int_0^r C_a(u)\, du = r \left\{ \frac{1}{a} \int_0^a \beta(u)\, du - \frac{1}{r} \int_0^r \beta(u)\, du \right\}, \qquad r < a,$$

we see that $F'_a(r) \geqslant 0$ if $r < a$ and $F'_a(r) = 0$ if $r \geqslant a$. Hence, $\operatorname{osc}(F_a) = \sup F_a - \inf F_a = \sup F_a = F_a(a)$.

(c) Next, since $C_a(a) = \gamma(a) - \beta(a) \leqslant 0$, C_a may not be continuous at a. For this, we need a modification of C_a. Let $\varepsilon \in (0, a)$ and define

$$C_a^\varepsilon(r) = \begin{cases} C_a(r) - C_a(a)\, \dfrac{\varepsilon - r}{\varepsilon}, & \text{if} \quad r \in [0, \varepsilon] \\[2ex] C_a(a) \left(1 - \dfrac{r - a}{\varepsilon}\right), & \text{if} \quad r \in [a, a + \varepsilon] \\[2ex] C_a(r), & \text{otherwise,} \end{cases}$$

$$F_a^\varepsilon(r) = \int_0^r ds \int_0^s C_a^\varepsilon(u)\, du.$$

Then $C_a^\varepsilon \in C(\mathbb{R}_+)$ and $F_a^\varepsilon \in C^2(\mathbb{R}_+)$. Moreover, it is not difficult to check that $(F_a^\varepsilon)' \geqslant 0$, $(F_a^\varepsilon)'(r) = 0$ for all $r \geqslant a + \varepsilon$ and $C_a^\varepsilon(r) - (1/r) \int_0^r C_a^\varepsilon(u)\, du \leqslant 0$ (Note that $\int_0^a C_a(r)\, dr = 0$). Hence $\operatorname{osc}(F_a^\varepsilon) = \sup F_a^\varepsilon = F_a^\varepsilon(a + \varepsilon) \to F_a(a)$ as $\varepsilon \to 0$.

(d) Take $V_\varepsilon(x) = F_a^\varepsilon(\rho(x))$, where $\rho(x) = \rho(p, x)$. Then $\operatorname{osc}(V_\varepsilon) = F_a^\varepsilon(a + \varepsilon)$. On the other hand, for $x \in M$ and $X \in T_x M$ with $\|X\| = 1$, by (2.1), we have

$$\begin{aligned} \operatorname{Hess}_{V_\varepsilon}(X, X) &= (F_a^\varepsilon)'(\rho) \operatorname{Hess}_\rho(X, X) + (F_a^\varepsilon)''(\rho)(X\rho)^2 \\ &\geqslant \frac{1}{\rho} \int_0^\rho C_a^\varepsilon(u)\, du + \left[C_a^\varepsilon(\rho) - \frac{1}{\rho} \int_0^\rho C_a^\varepsilon(u)\, du \right] (X\rho)^2 \\ &\geqslant C_a^\varepsilon(\rho). \end{aligned}$$

Here in the last step, we have used the fact that $(X\rho)^2 \leqslant \|X\|^2 = 1$ and $C_a^\varepsilon(\rho) - (1/\rho)\int_0^\rho C_a^\varepsilon(u)\,du \leqslant 0$. Therefore,

$$\inf_{x \in M} K(V - V_\varepsilon, x) \geqslant \inf_{r \geqslant 0} \{C_a^\varepsilon(r) + \beta(r)\} \geqslant \gamma(a).$$

By the B.-E. criterion and (1.2) we obtain $\alpha(V) \geqslant \gamma(a) \exp[-F_a^\varepsilon(a+\varepsilon)]$. Then (2.3) follows by letting $\varepsilon \to 0$.

(2) The proof of part (2) of Theorem 1.3 is similar. Recall that the functions γ and F_a are given by (1.4) with $f(r) = \sin(\sqrt{k}\,r)/\sqrt{k}$. By using the smoothing approximation as in the proof (c) above, we may and will assume that F_a is a C^2-function: Next, for $\rho(x) < a$, we have $F_a''(\rho) = f'(\rho)[\gamma(a) - \tilde{\beta} \circ f(\rho)] \geqslant f'(a)\,\gamma(a) - \beta(\rho)$. Thus, as we did in proof (d),

$$\mathrm{Hess}_{F_a(\rho)}(X, X) = F_a'(\rho)\,\mathrm{Hess}_\rho(X, X) + F_a''(\rho)(X\rho)^2 \geqslant f'(a)\,\gamma(a) - \beta(\rho).$$

Therefore, $K(V - F_a(\rho), x) \geqslant f'(a)\,\gamma(a)$ for $\rho(x) < a$. On the other hand, since $F_a(\rho) = F_a(a)$ for all $\rho > a$, we have $K(V - F_a(\rho), x) = K(V, x) \geqslant \beta(a) \geqslant f'(a)\,\tilde{\beta} \circ f(a) \geqslant f'(a)\,\gamma(a)$ for $\rho(x) \geqslant a$. Now, the desired conclusion follows from the B.-E. criterion and (1.2). ∎

In view of the proofs of Theorems 1.1 and 1.3, one may expect some further improvement. For instance, one may take $-k$ into account when $k < 0$. In part (1) of Theorem 1.3, one may use $h \circ \rho$ instead of ρ for some suitable function h. However, on the one hand, we restrict ourselves to general and computable estimation. Based on this and also from the geometric point of view, our perturbing potentials are more or less natural. On the other hand, we have tried several different potentials, including the above suggestions, but none of them ever produces a better estimate.

Proof of Corollary 1.4. Consider the operator $\bar{L} = \sum_{i,j=1}^d (\sigma^2)_{ij} [(\partial^2/\partial x_i \partial x_j) + (\partial V/\partial x_j)(\partial/\partial x_i)]$ in $\mathbb{R}^d$. By (1.6), we have

$$\alpha(L) \geqslant \alpha(\delta \bar{L}) = \delta \alpha(\bar{L}). \tag{2.6}$$

On the other hand, under the Riemannian metric $g(\partial/\partial x_i, \partial/\partial x_j) = (\sigma^2)_{ij}^{-1}$, we have $\bar{L} = \Delta_g + \nabla_g V$ (see [3]). For $x \in \mathbb{R}^d$ and $X \in T_x\mathbb{R}^d$ with $g(X, X) = 1$, there exists $c \in \mathbb{R}^d$ such that $X = \sum_i^d c_i \partial/\partial x_i$ and $c^*(\sigma^{-1})^2 c = 1$. Then

$$\mathrm{Hess}_V(X, X) = \sum_{i,j=1}^d c_i c_j \frac{\partial^2 V}{\partial x_i \partial x_j} = (\sigma^{-1}c)^* \left[\sigma \left(\frac{\partial^2 V}{\partial x_i \partial x_j}\right) \sigma\right] (\sigma^{-1}c) \leqslant \lambda_V(x).$$

Hence $K(V, x) = -\lambda_V(x)$ and so Corollary 1.4 follows from (2.6) and Theorem 1.3 (1). ∎

Proof of Theorem 1.5. (a) As usual, one uses the Riemannian metric $g(\partial/\partial x_i, \partial/\partial x_j) = \bar{a}(x)^{-1}$ instead of the Euclidean one I. Note that the induced Riemannian distance is indeed equivalent to the Euclidean one since $\bar{v}_1 I \leqslant \bar{a}(x) \leqslant \bar{v}_2 I$. Thus, without loss of generality, we may and will assume that $\bar{a}(x) \equiv I$.

(b) Given $g \in C^1(\mathbb{R}^d)$ with compact support, let $f = g e^{u/2}$, where $u = -V + \log Z$. By (1.6), we have

$$\int g^2 \log(g^2 e^u)\, dx - \left(\int g^2\, dx\right) \log\left(\int g^2\, dx\right)$$
$$\leqslant \frac{2}{\alpha(L)} \int v \left(\|\nabla g\|^2 + \frac{1}{4} g^2\, \|\nabla V\|^2 + g\, \|\nabla g\|\, \|\nabla V\| \right) dx.$$

Equivalently,

$$\int g^2 \log g^2\, dx - \left(\int g^2\, dx\right) \log\left(\int g^2\, dx\right)$$
$$-\frac{2}{\alpha(L)} \int v (g\, \|\nabla g\|\, \|\nabla V\| + \|\nabla g\|^2)\, dx$$
$$\leqslant \int u g^2 \left(\frac{\|\nabla V\|^2\, v}{2\alpha(L)\, u} - 1 \right) dx. \tag{2.7}$$

(c) To prove the assertion, it suffices to construct a sequence $g_n \in C^1(\mathbb{R}^d)$ with compact support such that $\int u g_n^2 = 1$ and moreover the left side of (2.7) goes to zero as $n \to \infty$. To see this, assume that $\frac{1}{2} \overline{\lim}_{|x| \to \infty} [-\|\nabla V(x)\|^2\, v(x)/V(x)] =: A < \infty$. Then in the limit (2.7) yields $0 \leqslant \alpha(L)^{-1} A - 1$. The construction given below is a slight modification from [9]. Choose a non-negative $h \in C^1(\mathbb{R})$ with support $[0, 1]$, $\int_0^1 h(s)^2\, ds = 1$ and $\inf\{h(s) : s \in [0.1, 0.9]\} = 1$. Define

$$\ell_n = \int_{\{n \leqslant |x| \leqslant 2n\}} h\left(\frac{|x| - n}{n}\right) dx, \qquad g_n(x) = \frac{1}{\sqrt{\ell_n u(x)}}\, h\left(\frac{|x| - n}{n}\right).$$

Then g_n is well defined for large n and has support $\{x : n \leqslant |x| \leqslant 2n\}$.

(d) Let $\bar{\gamma}_n = \gamma_n + \log Z$, then for large n and $|x| \geqslant n$ we have

$$\|g_n\|_\infty \leqslant \frac{1}{\sqrt{\ell_n \bar{\gamma}_n}} \|h\|_\infty, \qquad \|\nabla g_n\| \leqslant \frac{\|\nabla h\|_\infty}{n \sqrt{\ell_n \bar{\gamma}_n}} + \frac{\|\nabla u\|\, \|h\|_\infty}{2u \sqrt{\ell_n \bar{\gamma}_n}}. \tag{2.8}$$

On the other hand,

$$\|\nabla u(x)\|\, v(x) \leqslant 3AC\,|x| \qquad \text{and} \qquad -\frac{\|\nabla u(x)\|^2\, v(x)}{V(x)} \leqslant 3A \tag{2.9}$$

for large $|x|$. So for large n,

$$\begin{aligned}\|\nabla u\|\ \|\nabla g_n\|\ v g_n &\leqslant \left\{ \|h\|_\infty\ \|\nabla h\|_\infty \frac{3AC\,|x|}{n\ell_n \bar{\gamma}_n} + \frac{3A\ \|h\|_\infty^2}{2\ell_n \bar{\gamma}_n} \right\} I_{\{n \leqslant |x| \leqslant 2n\}} \\ &\leqslant \frac{C_1}{\ell_n \bar{\gamma}_n} I_{\{n \leqslant |x| \leqslant 2n\}}\end{aligned}$$

for some constant $C_1 > 0$. Note that $\ell_n \geqslant \int_{\{1.1n \leqslant |x| \leqslant 1.9n\}} dx \geqslant C_2 \int_{\{n \leqslant |x| \leqslant 2n\}} dx$ for some constant $C_2 > 0$ (Here is the main place in which the restriction on the growth of the volume is required). We obtain

$$\lim_{n \to \infty} \int \|\nabla u\|\ \|\nabla g_n\|\ v g_n\, dx \leqslant \lim_{n \to \infty} \frac{C_1}{\bar{\gamma}_n C_2} = 0. \tag{2.10}$$

Next, by the second inequality of (2.9) and the assumption, we have

$$v(x) \leqslant \frac{3A}{-V} \left(\frac{|V|}{\|\nabla u\|} \right)^2 \leqslant \frac{3AC^2\,|x|^2}{-V} \leqslant \frac{4AC^2\,|x|^2}{\bar{\gamma}_n}$$

for $|x| \in [n, 2n]$ and large n. Moreover,

$$\frac{v\,\|\nabla u\|^2}{u^2 \ell_n \bar{\gamma}_n} = \frac{\|\nabla u\|^2\, v}{|u|} \cdot \frac{1}{|u|\ \ell_n \bar{\gamma}_n} \leqslant \frac{3A}{\ell_n \bar{\gamma}_n^2}.$$

Combining these two estimates with the second inequality of (2.8), we obtain

$$\lim_{n \to \infty} \int v\, \|\nabla g_n\|^2\, dx = 0. \tag{2.11}$$

(e) Since $g_n^2 \leqslant \|h\|_\infty\, (\ell_n \bar{\gamma}_n)^{-1}\, I_{\{n \leqslant |x| \leqslant 2n\}}$, we have $\int g_n^2 \leqslant \|h\|_\infty / (C_2 \bar{\gamma}_n) \to 0$ as $n \to \infty$ and so

$$\lim_{n \to \infty} \left(\int g_n^2\, dx \right) \log \left(\int g_n^2\, dx \right) = 0 \tag{2.12}$$

Finally, noticing that $g_n^2 \leqslant \|h\|_\infty/(\ell_n \bar{\gamma}_n) < e^{-1}$ for large n, $|x \log x|$ is increasing in $(0, e^{-1})$ and $\ell_n \leqslant C_3 n^d$ for some $C_3 > 0$, we have

$$\left| \int g_n^2 \log g_n^2 \, dx \right| \leqslant \int_{\{n \leqslant |x| \leqslant 2n\}} \frac{\|h\|_\infty}{\ell_n \bar{\gamma}_n} \left| \log \frac{\|h\|_\infty}{\ell_n \bar{\gamma}_n} \right| dx$$

$$\leqslant \left| \frac{\|h\|_\infty}{C_2 \bar{\gamma}_n} \log \frac{\|h\|_\infty}{\bar{\gamma}_n} \right| + \frac{\|h\|_\infty}{C_2 \bar{\gamma}_n} (d \log n + \log C_3)$$

which goes to zero as $n \to \infty$. Combining this with (2.10)–(2.12), the assertion follows from (1.6) by letting $n \to \infty$. ∎

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